NPT Dynamics, Minimization and Elastic Constants for Triclinic Cells

New LAMMPS features briefs
LAMMPS Users’ Workshop @ CSRI
Thursday, Feb 25, 2010, 3:15 p.m.

Aidan Thompson
Sandia National Labs
Parrinello-Rahman MD

Invented by:
   Parrinello and Rahman, J. Appl. Phys. 52 7182
   (1981) (1,268 citations up to Feb 2010)

Core Ideas:
1. They introduced the periodic cell matrix as additional coordinates. They also expressed the strain energy in terms of this matrix:

\[ E = U + P_t (V - V_0) + E_{strain} \]

\[ E_{strain} = \sigma_t : \epsilon = \frac{1}{2} V_0 \text{Tr} h^{-1}_0 \sigma_t (h^{-1}_0)^t h^t h \]
New *NVT, NpT, NpH, NσT* Fixes

- Nose-Hoover chain thermostat for particle velocities
- Nose-Hoover chain thermostat for barostat “velocities”
- Barostat coupling styles:
  - Isotropic
  - Anisotropic
  - Triclinic (Parrinello-Rahman)
- Barostat “pressure” styles
  - Scalar hydrostatic pressure
  - Tensorial non-hydrostatic stress
- Martyna-Tobias-Klein correction to Nose-Hoover barostat
New NVT, NPT, NPH Fixes

**NVT Ensemble**
fix 1 all nvt temp 300.0 300.0 100.0

**NpT Ensemble**
fix 1 water npt temp 300.0 300.0 100.0 &
iso 0.0 0.0 1000.0

**NpH Ensemble, anisotropic orthorhombic box**
fix 1 water nph aniso 0.0 0.0 1000.0

**NpT Ensemble, Parrinello-Rahman**
fix 2 jello npt temp 300.0 300.0 100.0 &
tri 5.0 5.0 1000.0
New NVT, NPT, NPH Fixes

$N\sigma T$ Ensemble, Parrinello-Rahman

fix 3 ice    npt    temp 273.15 273.15 &
            x 0.0 1.0 0.5 &
            y 0.0 2.0 0.5 &
            z 0.0 3.0 0.5 &
            yz 0.0 0.1 0.5 &
            xz 0.0 0.2 0.5 &
            xy 0.0 0.3 0.5
Example: Strained FCC Nickel

```plaintext
fix       mynpt all npt &
pchain 3 tchain 3 mtk yes &
temp 300.0 300.0 0.1 &
x  10000.0  10000.0 1.0 &
y  40000.0  40000.0 1.0 &
z  80000.0  80000.0 1.0 &
xy -10000.0 -10000.0 1.0 &
xz -20000.0 -20000.0 1.0 &
yz -30000.0 -30000.0 1.0 &
```
Elastic Constants, Nickel, $P_{xx} = -5$ GPa, $T = 300$ K

$$C^{-1}_{ijkl} = S_{ijkl} = \beta V_0 \left< \epsilon_{ij} \epsilon_{kl} \right>$$

![Graph of Elastic Constants vs Timesteps](graph1)

![Graph of Elastic Constants vs Timesteps](graph2)
Triclinic Cell Relaxation

\[ P = 0 \]

```
fix 1 all box/relax xyz 0.0 vmax 0.001
```

\[ L_{xx}, L_{yy} \text{ fixed, } P_{zz} = 1000 \text{ atm.} \]

```
fix 1 water box/relax aniso NULL NULL 1000.0
```

Non-hydrostatic target stress tensor

```
fix 3 ice box/relax tri 10.0 20.0 30.0 0.0 0.0 0.0 10.0 &
nreset_ref 1000
```
Triclinic Cell Relaxation

Non-hydrostatic target stress tensor

```plaintext
fix 1 all box/relax tri 10000.0 40000.0 80000.0 &
    -10000.0 -20000.0 -30000.0 &
    nreset_ref 10

min_modify dmax 1.0e-2 line quadratic
minimize 0.0 1.0e-10 100 200
```
Elastic Constants, $T = 0$
LJ FCC crystal uniaxial strain

variable dneg equal -$\{up\}*\{ylen\}$
displace_box all xy delta $\{dneg\}$

: variable C66neg equal ($\{pxy\}-\{pxy0\}$)/$\{up\}$
Effect of Linesearch on Elastic Constant

![Graph showing the effect of linesearch on elastic constant. The graph plots strain on the x-axis and elastic constant $C_a$ (eV/A³) on the y-axis. The graph compares Backtrack linesearch (marked with X) and Quadratic Linesearch (marked with O). The graph shows a decrease in $C_a$ as strain increases.](image-url)
Summary

- Nose-Hoover chain thermostats
- Parrinello-Rahman dynamics for $NpT$ and $N\sigma T$
- Triclinic Box Relaxation for target $p$ or $\sigma$
- Elastic constants:
  - $T=0$, $p \neq 0$ or $\sigma \neq 0$ easy
  - $T > 0$ hard